CSCI 1470/2470
Spring 2023

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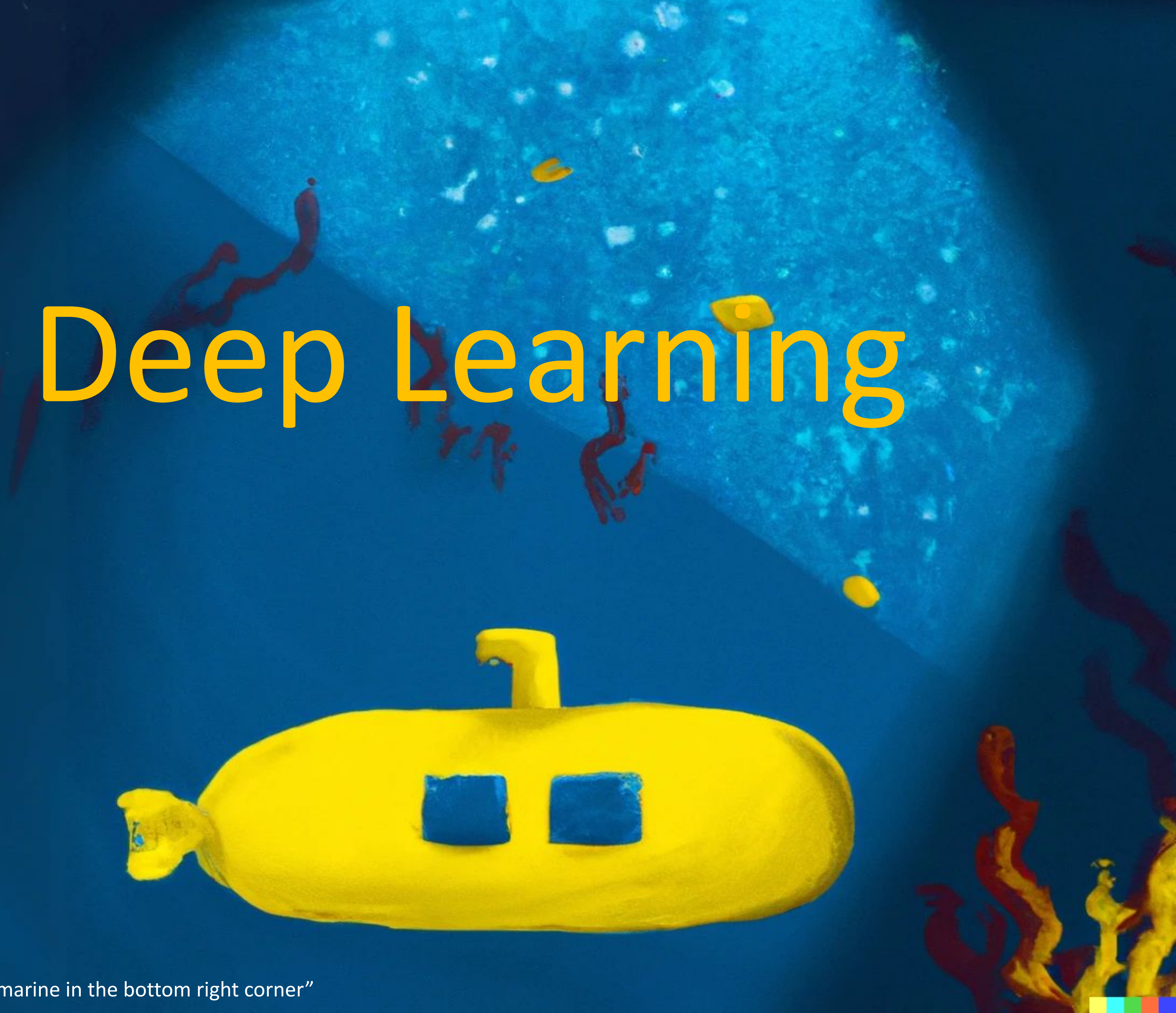
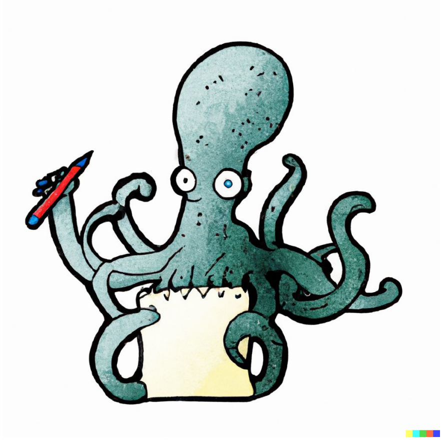
February 27, 2023
Monday

Deep Learning



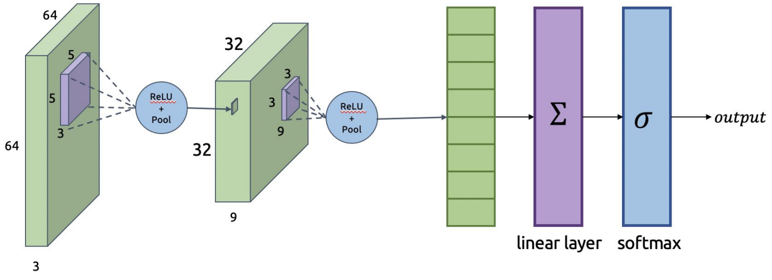
DALL-E 2 prompt “a painting of deep underwater with a yellow submarine in the bottom right corner”

Recap



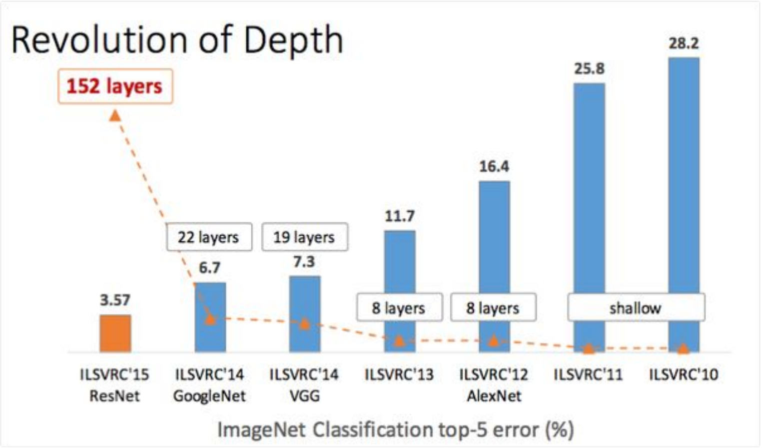
CNNs

- Architecture
- AlexNet + Pooling
- CNNs are “sort of” translationally invariant



Deeper CNNs

- Many layers = vanishing gradient
- ResNet + Residual blocks
- Batch normalization



MNIST & CIFAR are really nice datasets!

- There’s a clear “absolute truth”
  - A 4 is a 4, and a 5 is a 5
- Labels are guaranteed to be good
- Each class is well-represented – there’s lots of data for each class
- Lots of data in general

...most data isn't so nice

Examples of messy data

IMDB Movie Review Data

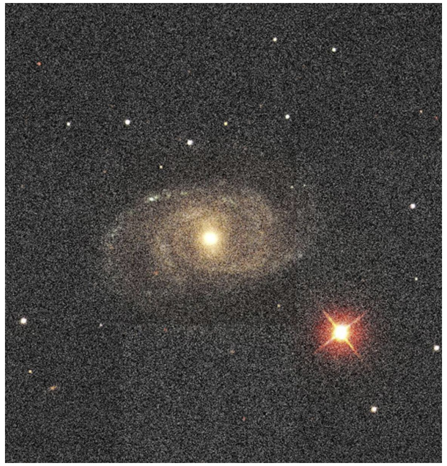
In the training set	In the test set
1. there is some ***great*** buddhist wisdom in this movie. ...whereas other biographies of famous people tend to get very poor this movie always stays focused and gives a ***good*** and ***honest*** portrayal of the dalai lama. all things being equal, it is a ***great*** movie, and i really ***enjoyed*** it. (The rating is 10.) 2. this is a ***great*** movie! it is so ***funny***. the love-story is ***excellent!*** i saw this movie when i was a kid and saw it again the other day. it's just as ***good***. robert zemeckis has made a wonder of an 80s movie. it's just ***superb***. ***watch it! watch it! watch it! highly recommended*** a long with a movie like raiders of the lost ark. (The rating is 10.) 3. i thought this was a very ***funny*** movies in the 80s style although it was finished in 1991. perhaps the title is a bit ***stupid*** and difficult to remember. ...and all in all this movie is a ***great*** view into a time before the home computer got customary, internet, cell phones and so forth. moreover, the old lady who plays the babysitter is really ***funny***. (The rating is 8.)	this is a ***stunningly beautiful*** movie. the music by phillip glass is just a work of pure genius. i can watch this movie ***again and again***. ... how was it filmed? it 's so ***amazing***. if you have not seen this film watch it - ***again and again***! this must be the only movie which in a ***powerful*** way, ... ***watch it! watch it! watch it!*** (The rating is 10.)

Patient Data

Family No.	Patient	Gender/Age of onset (year)	Clinical findings	Mutation site	*PHEX* mutation	Inheritance
1	(II-2) daughter	F/3	Retarded dentition	Exon 20	Trp660X (c.1980G>A)	Familial
1	(I-1) father	M/1.5	Genu varum	Exon 20	Trp660X (c.1980G>A)	Familial
2	(II-1) daughter	F/2	Genu varum; retarded dentition	**Exon 17**	**His584Pro (c.1751A>C)**	Familial
2	(I-2) mother	F/1.5	Genu varum; retarded dentition; odontodysplasia; teeth falling out	**Exon 17** **Exon 11**	**His584Pro (c.1751A>C)** **Gly395Arg (c.1183G>C)**	Familial
3	(II-2) daughter	F/4	Genu varum and bone pain	Exon 12	Trp444X (c.1332 G>A)	Familial
3	(I-2) mother	F/5	Hip and knee joint pain; kyphosis; bone pain	Exon 12	Trp444X (c.1332 G>A)	Familial
4	(III2) son	M/1.5	Genu varum	Intron 15	c.1646-2A>T	Familial
4	(II2) mother	F/2	Genu varum	Intron 15	c.1646-2A>T	Familial
4	(I2) grandmother	F/5	Genu varum	Intron 15	c.1646-2A>T	Familial
5	(II1) son	M/5	Genu varum (mild); bone pain; growth retardation	Intron 10	c.1174-1G>A	Familial
5	(I2) mother	F/4	Genu varum; odontodysplasia; teeth falling out; growth retardation	Intron 10	c.1174-1G>A	Familial
6	(II1) daughter	F/2	Bowing of legs	Exon 16	Tyr565Phefsx5 (c.1694delA)	Familial
6	(I2) mother	F/2	Bowing of legs	Exon 16	Tyr565Phefsx5 (c.1694delA)	Familial
7	(III1) son	M/0.75	Genu varum; hip pain; growth retardation	Intron 17	c.1768+2T>G	Sporadic
8	(III1) son	M/1.5	Genu varum; cephalus quadratus	Exon 21	Trp692IlefsX2 (c.2077_*4delinsA)	Sporadic
9	(III1) daughter	F/1.3	Genu varum	Exon 15	Arg549X (c.1645C>T)	Sporadic

Footnotes: Novel mutations are bolded.
doi:10.1371/journal.pone.0097830.t002

Astronomy data



DNA sequence data

```
>gi|1370453229|ref|XM_005245209.2|:1-809 PREDICTED: Homo sapiens NADH:ubiquinone
oxidoreductase core subunit S2 (NDUFS2), transcript variant X1, mRNA
GTAGGTTCGGGAAGCCTGGAGGATGTCAGGGTCACCCACAGAGGACCTCCACTCCCCCATCTGGGATGAG
GTGGCTCCTACACACCCCGACACTCCCCTCCGCACCACCAATGCCGGCGGCCTTGGCATCCTATTCTTTT
TTGTTTTGGTTTGGCGGGAGCTCTCAGACCCGCCCAGCCCCACTTAGGCTCCTTTCTCCAATCTCAATTT
ATGACATCTGGAAATTAGCTGGCTTTCCCAACTCCTGTCTTTTGGATTCAGTGATGGGAAAGTAATTGGC
AAAGCCTGGGGCTACCCTATAAGGGCAGGGCTCAGATACAATCCGAGAGCAGGACTAAAGCATGAGGGCG
GCCAAGGCGGAAGGGAGTAGGGAAGGAAGCGCCGCGCGTTTCCAAGATACGCAGGCGGGCTCGGCGAGAG
AGCACGAAGTATCTGCCCCACGCAGGAACGGCAATTTTCCCTTGCTCGCTCCTAGAAAAGCCAGCCAGGA
GCTGTGGGAGGAAACGCCCTCAGTAAAGATGACCGCGGTCACTGTTATCTAAACGCAAGTGAAGCCGAGT
CACAGGACCCGGATGTTGTCAGTTCGACGGTAAACGACCCTGCCAGCTTCCAAGAGGGCGGCTTCACTGT
GCGAATAGGTGAGAAGCCAAGAAGGAGGCGCGCTGGAGTTACTTCCGCCCGGTTCTCCTTCCCGCAGTCT
GCAGCCGGAGTAAGATGGCGGCGCTGAGGGCTTTGTGCGGCTTCCGGGGCGTCGCGGCCCAGGTGCTGCG
GCCTGGGGCTGGAGTCCGATTGCCGATTCAGCCCAGCAG>gi|1370453229|ref|XM_005245209.2|:810-1000
```

Dealing with messy data: preprocessing

- Always necessary (unless it's preprocessed for you…)
- Goal: get messy, unstructured data into **usable** data for your model
    - Ultimately, data must be converted into **tensors** to be fed to your model
- What exactly you need to do is dataset- and context- dependent
    - Language models: tokenization, UNKing, ...
    - Quantify non-numerical entities (e.g. categories □ one-hot vectors)
    - Drop outliers?
    - Normalize/standardize inputs

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Does this mean there's a group your model systematically fails for?

Does your quantification make sense? What assumptions does it make about the world – e.g. gender binary or racial categories?

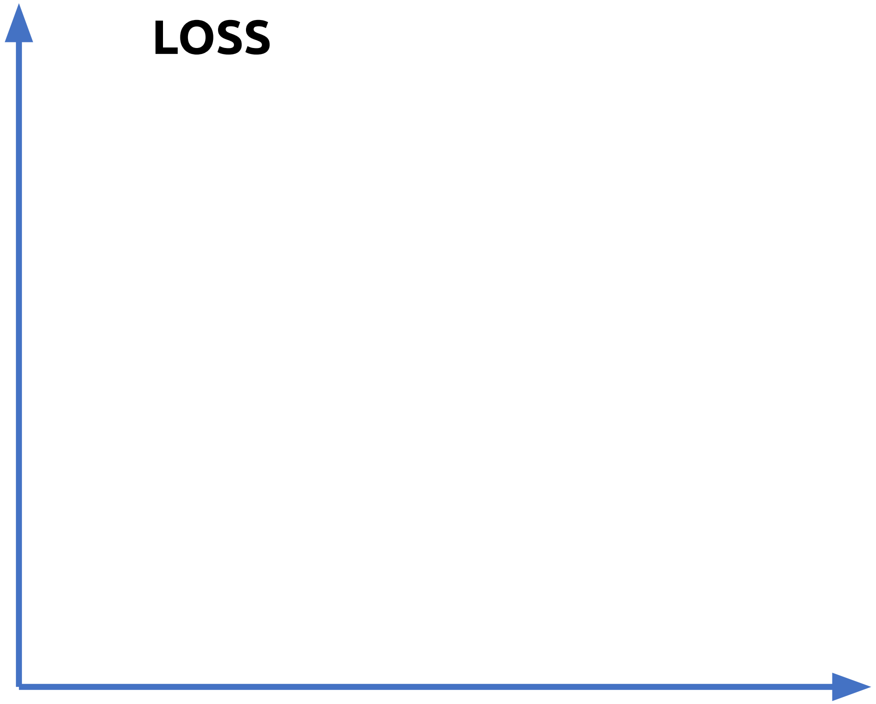
Consequences of complex data...

- Demo

Consequences of complex data...

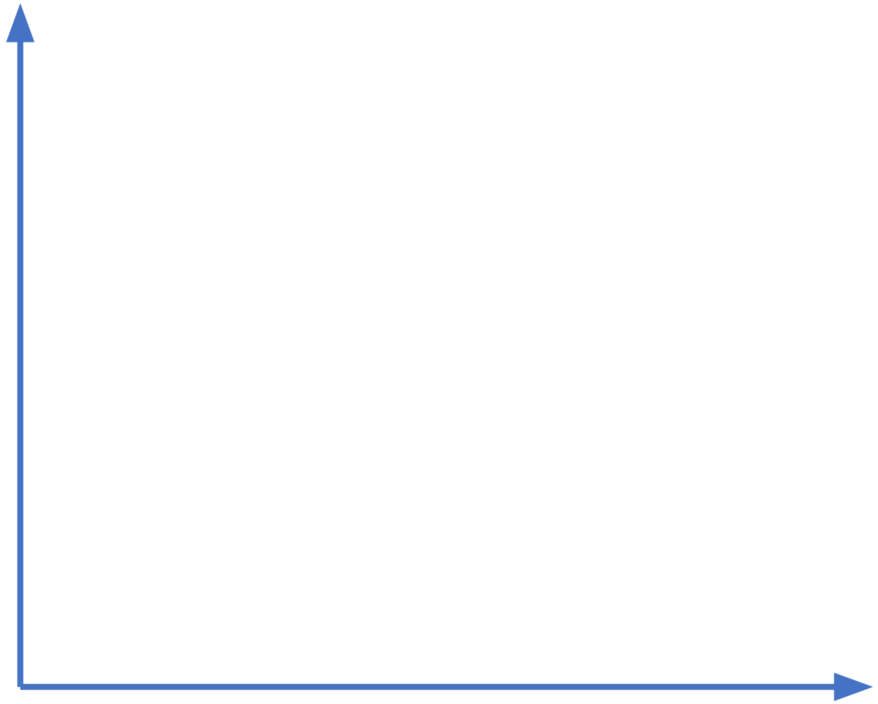
What is the simplest thing to do here?

MNIST – TRAINING LOSS
MNIST – VALIDATION LOSS



num_epochs

IMDB – TRAINING LOSS
IMDB – VALIDATION LOSS



num_epochs

This is an example of ***overfitting***

Overfitting: What can we do about it?

1. Early stopping

Early stopping: pseudocode

```
curr_valid_loss = inf
for i in range(n_epochs):
    train model()
    new_valid_loss = model.get_test_loss()
    if new_valid_loss > curr_valid_loss:
        break
    else:
        curr_valid_loss = new_valid_loss
```

Early stopping: thoughts

This is kind of a hack...

Can we stop validation loss from increasing altogether?

Any ideas?

Overfitting: What can we do about it?

1. Early stopping

2. Reduce parameters

Reduce parameters - why?

More parameters = more ‘knobs’ to fiddle = more possibilities to learn something overly-specific to the training data

- Example: curve fitting

Reduce parameters - why?

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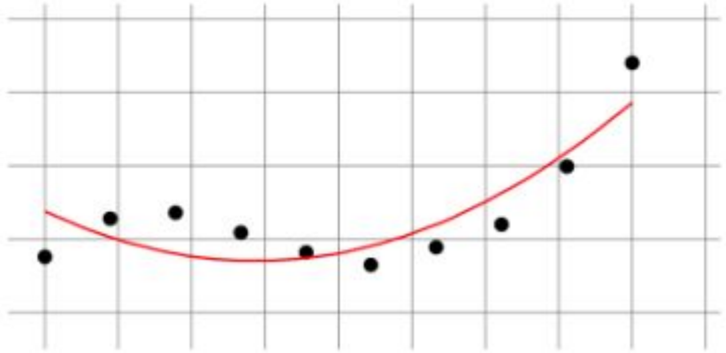
- Example: curve fitting

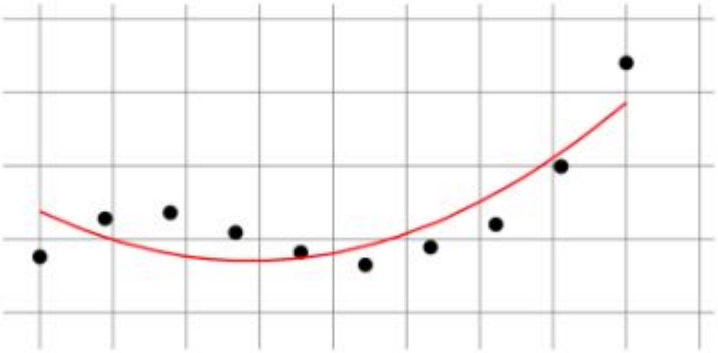


$$y = 3x^2 + 2x + 4$$

Reduce parameters - why?

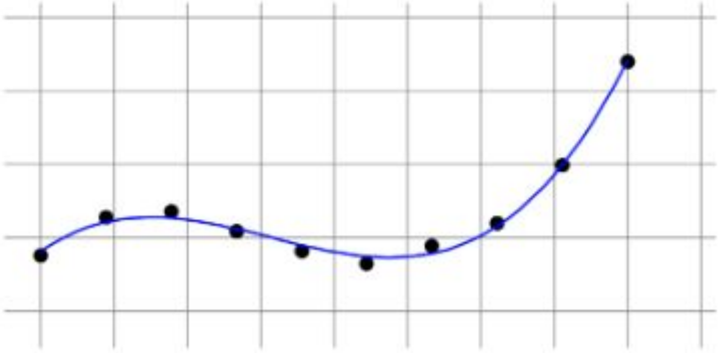
More parameters = more ‘knobs’ to fiddle = more possibilities to learn something overly-specific to the training data

- Example: curve fitting



Degree 2

$$y = 3x^2 + 2x + 4$$



Degree 3

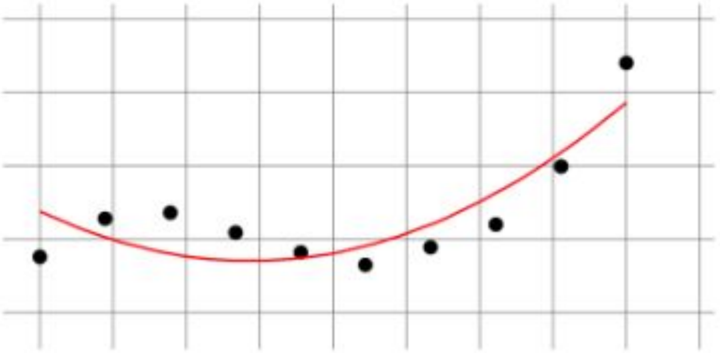
$$y = 2x^3 - 4x^2 + x - 3$$

Reduce parameters - why?

More parameters = more ‘knobs’ to fiddle = more possibilities to learn something overly-specific to the training data

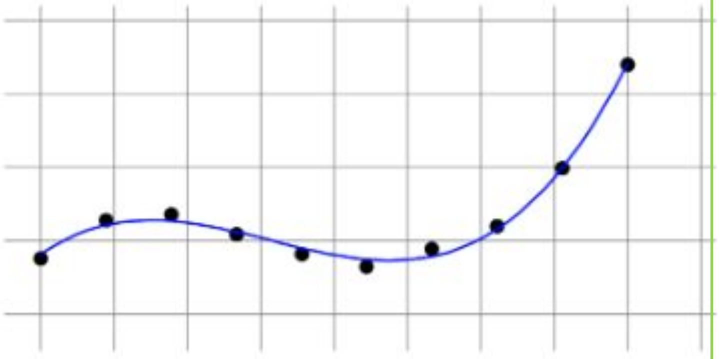
- Example: curve fitting

This is probably the best fit curve…



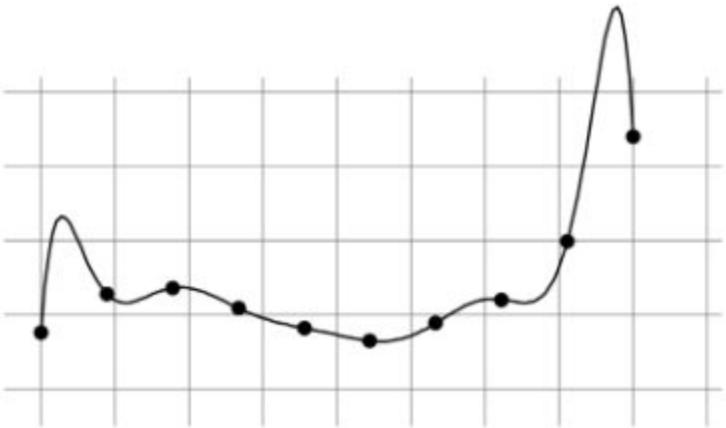
Degree 2

$$y = 3x^2 + 2x + 4$$



Degree 3

$$y = 2x^3 - 4x^2 + x - 3$$



Degree 10

$$y = 7x^{10} + x^9 + 6x^8 - 3x^7 - 2x^6 \ldots + x - 3$$

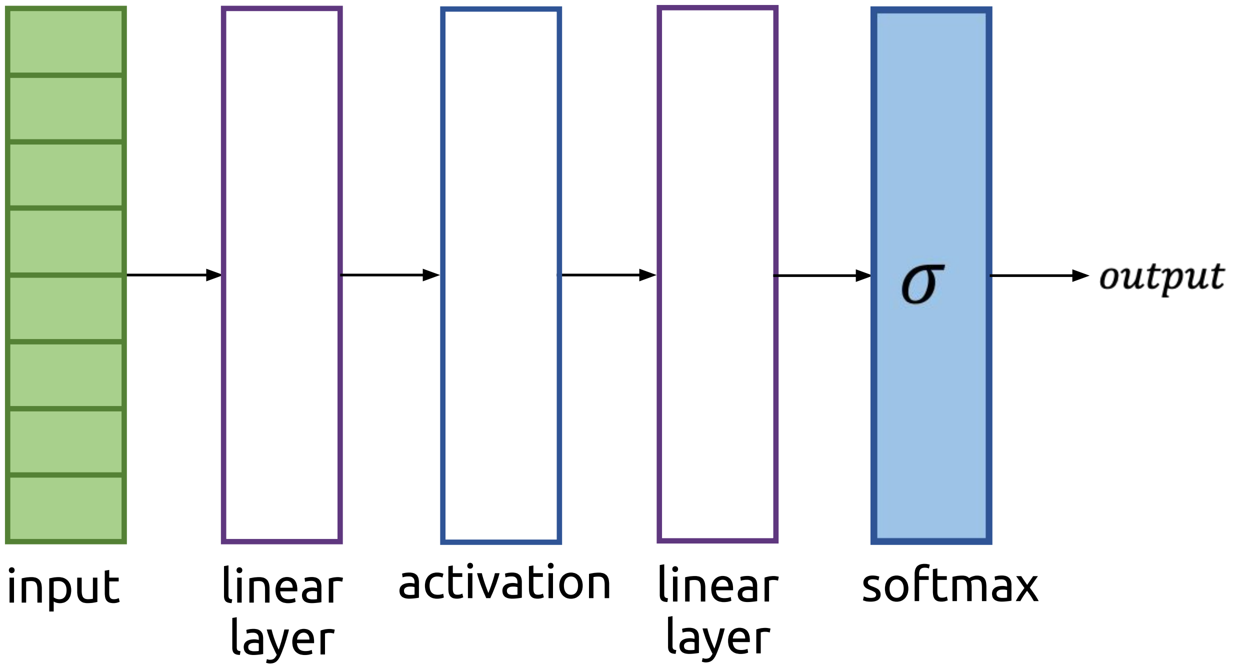
Reduce parameters in a Neural Net: How?

- Fully connected nets?
- CNN?
- ***Any*** NN?

Reduce parameters in a Neural Net: How?

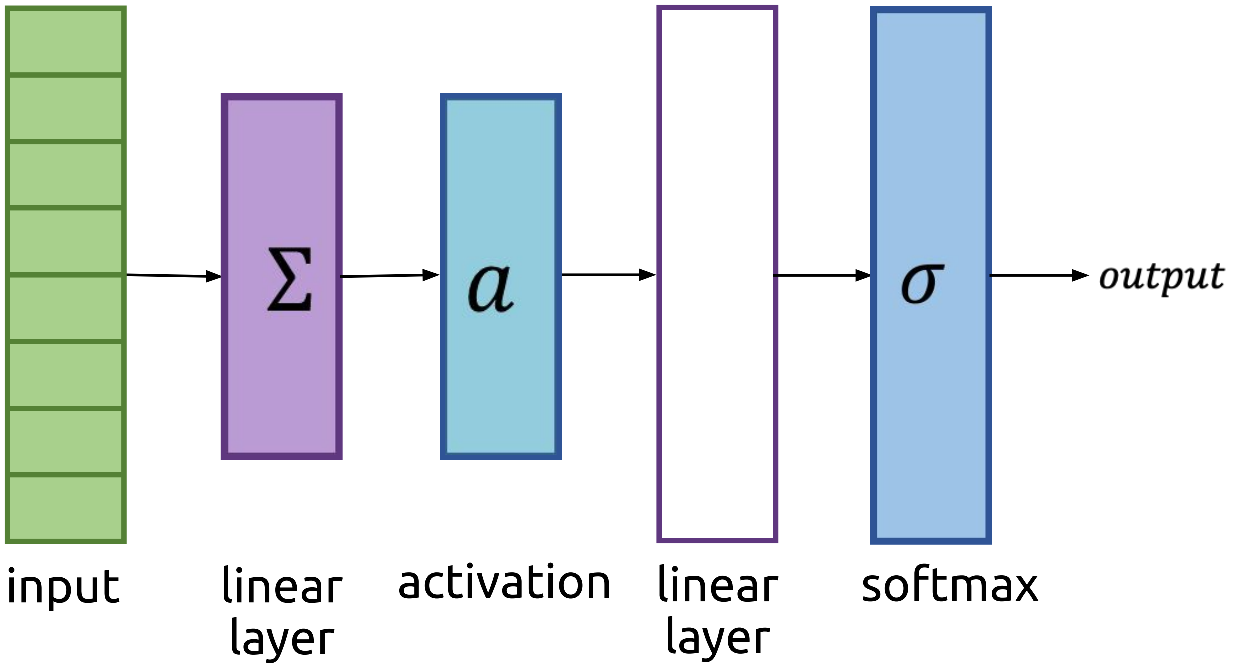
- Fully connected:

What can be done here?



Reduce parameters in a Neural Net: How?

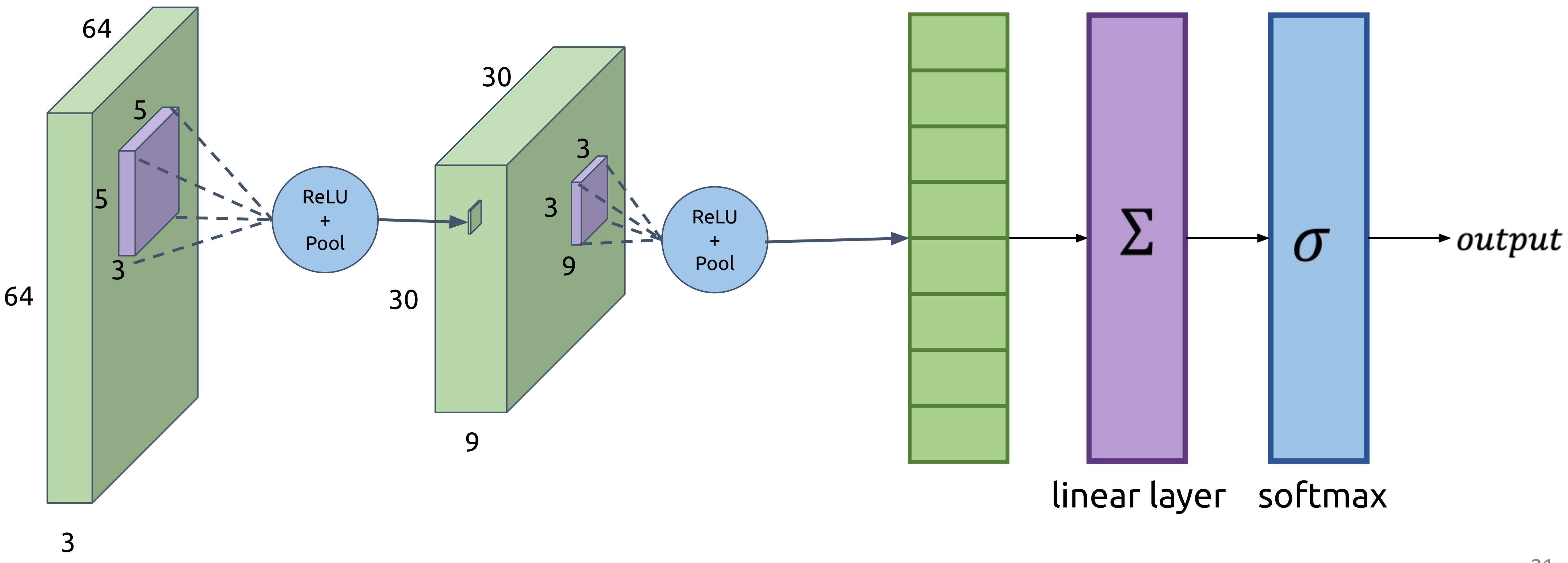
- Fully connected: reduce layer size



Reduce parameters in a Neural Net: How?

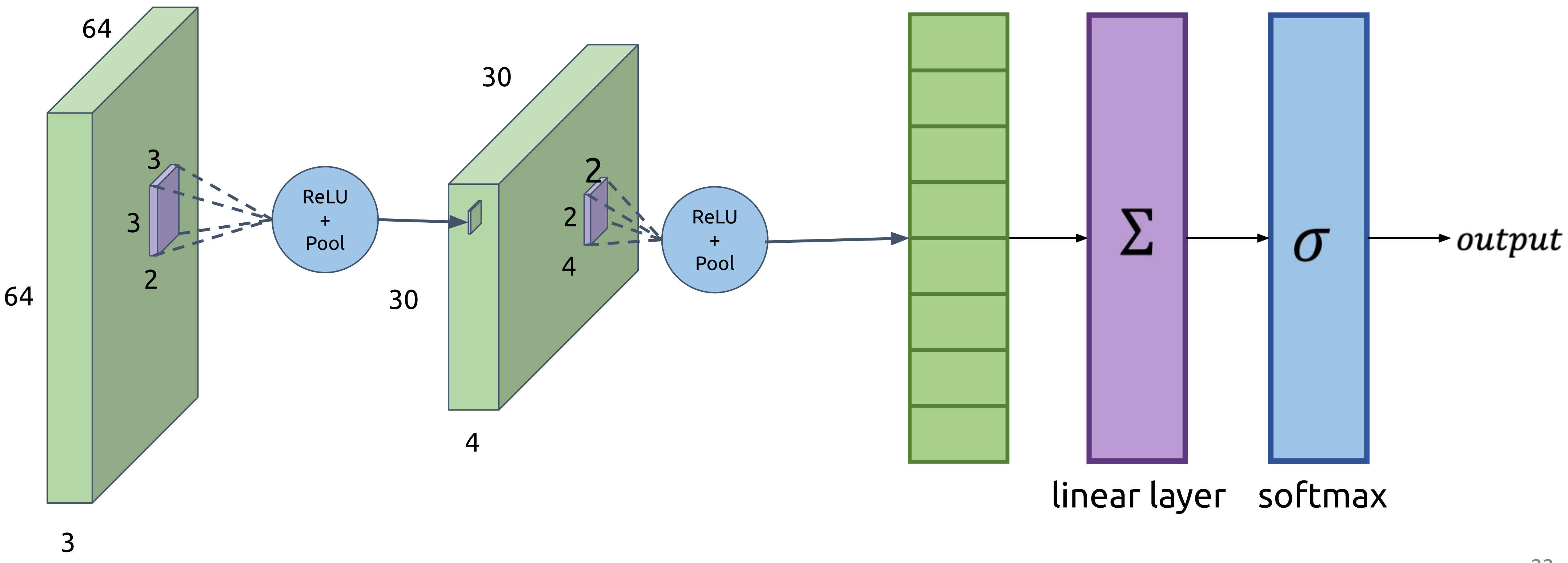
- CNN:

What about here?



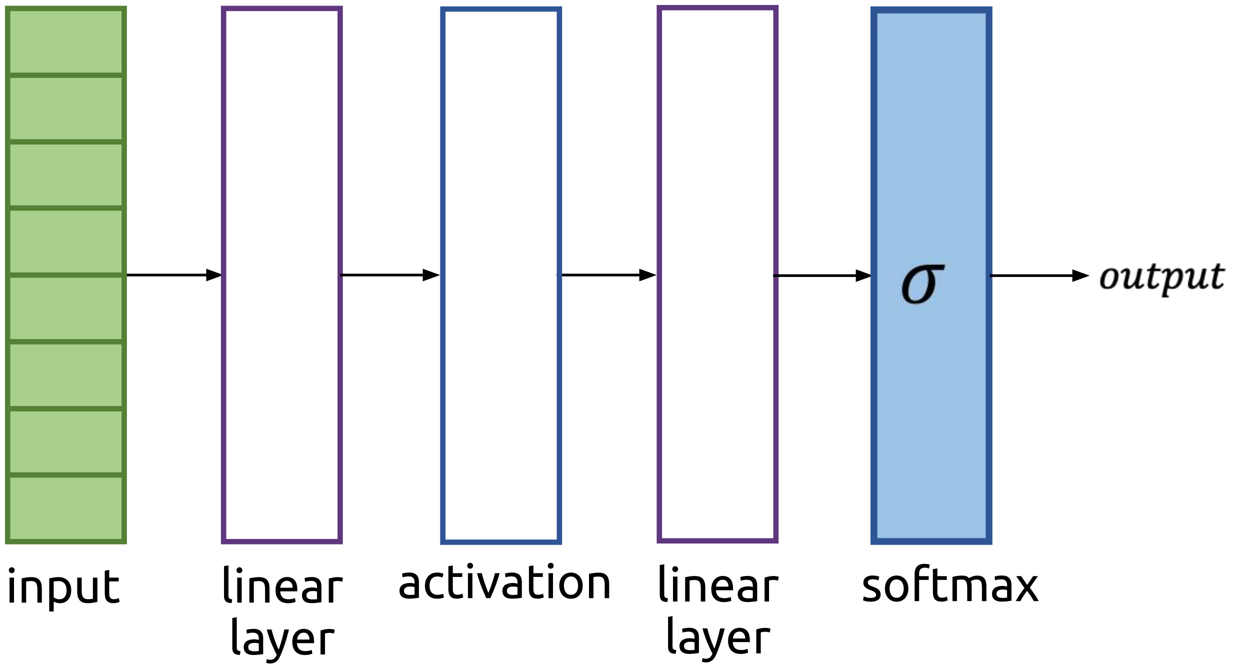
Reduce parameters in a Neural Net: How?

- CNN: decrease num_channels (and also possibly filter_size)



Reduce parameters in a Neural Net: How?

- All architectures: Decrease number of layers



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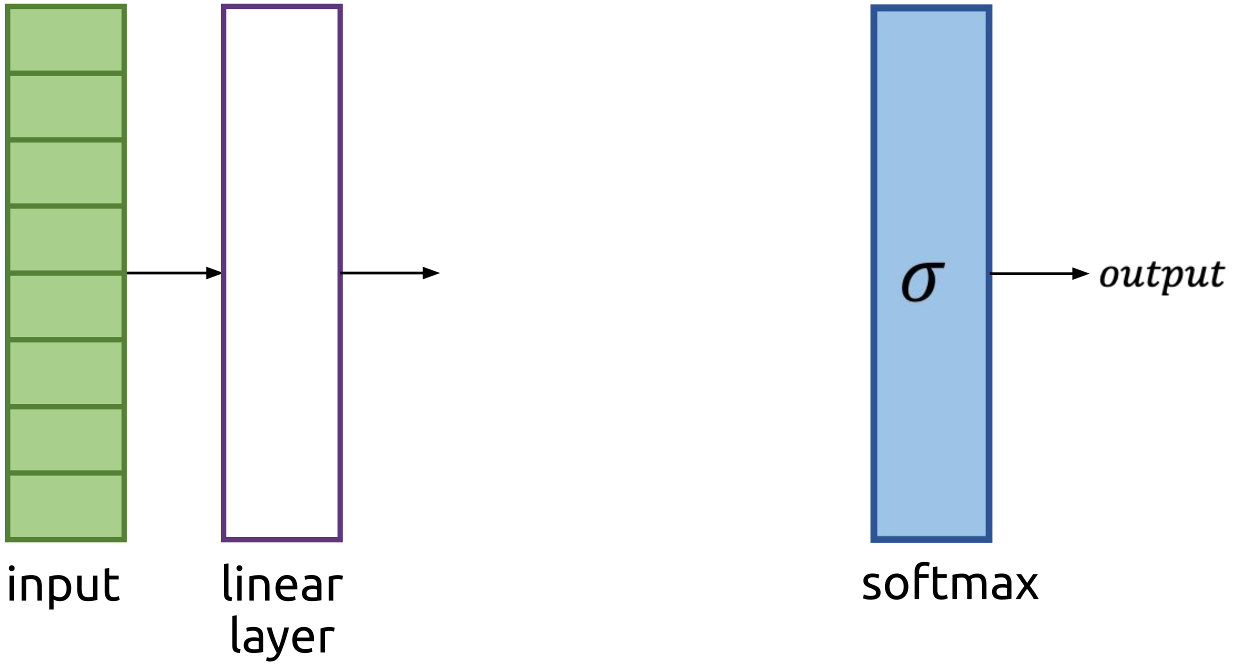

Reduce parameters in a Neural Net: How?

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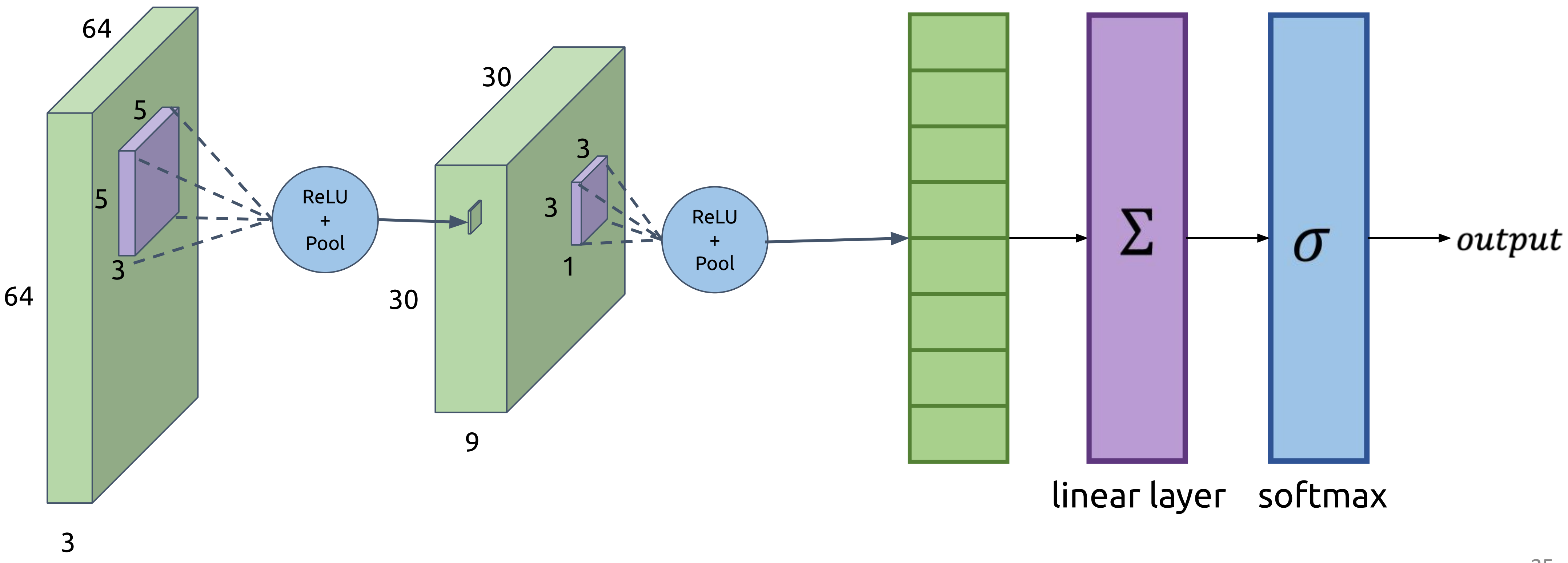
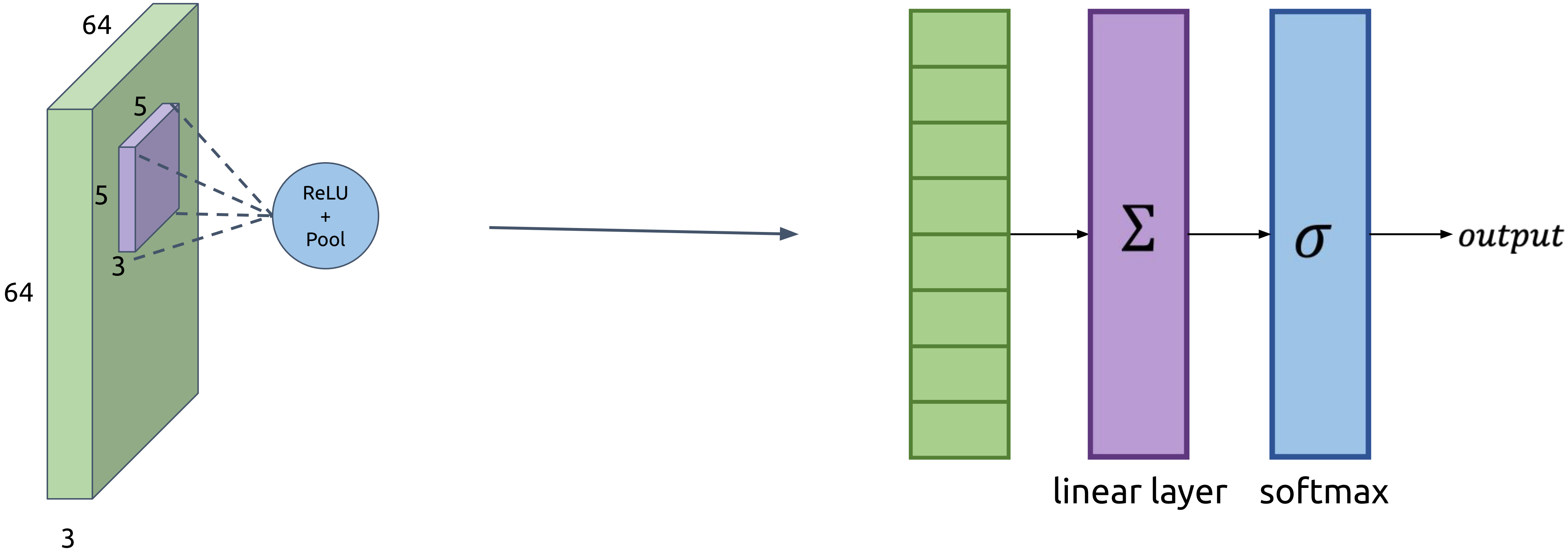


Reduce parameters in a Neural Net: How?

- All architectures: Decrease number of layers



Reducing parameters: Why not?

- Seen (by deep learning folks) as a bit ‘old-fashioned’
  - Classical perspective: model complexity should match data complexity
  - Deep learning perspective: all real-world data is infinitely complex (i.e. there are infinite variations on what a handwritten digit can look like). If your model is overfitting, that just means you don’t have enough data—so get more!
- What if we can’t get more data?
  - (e.g. it’s prohibitively expensive to gather more data)

Synthesize variations on your data

Overfitting: What can we do about it?

1. Early stopping
2. Reduce parameters
3. **Data augmentation**

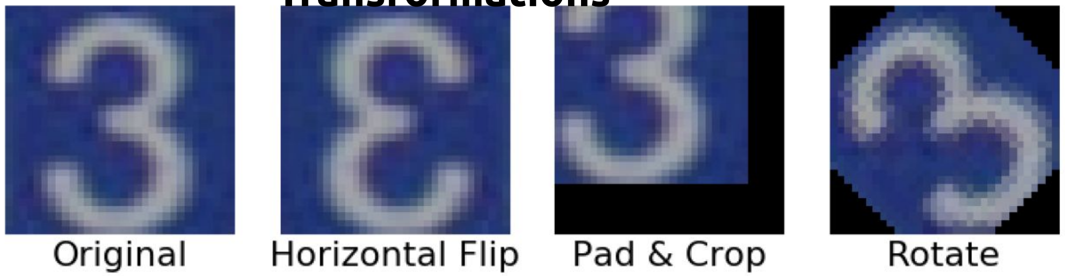
Data Augmentation

- Generate (random) variations on your training data, treat that as more training data
  - Assumption: your (random) variations still produce data that is within the expected distribution of training data (so you can't get ***too*** crazy)

- Most commonly used on image data

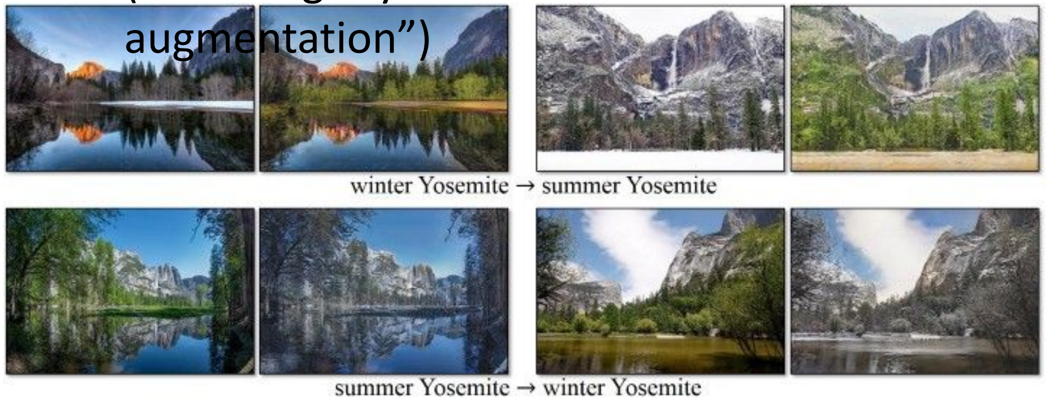
Data Augmentation: Image Examples

Geometric Transformations



https://bair.berkeley.edu/blog/2019/06/07/data_aug/

Fancy (Learned) Semantic Transforms
(i.e. “Image synthesis for data augmentation”)



https://junyanz.github.io/CycleGAN/

Filters & Pixel Intensity Transforms
Blur, sharpen, contrast adjust, …

https://towardsdatascience.com/data-augmentation-for-deep-learning-4fe21d1a4eb9

Data Augmentation: Limitations

- Your model might still overfit!
  - In general, it’s impossible to design an augmentation procedure that covers ***all*** the dimensions of variation your data might experience
  - Your model can still overfit to patterns in the dimensions that you don’t augment with variations...

Overfitting: What can we do about it?

1. Early stopping
2. Reduce parameters
3. Data augmentation
4. **Dropout**

Dropout – general intuition

- Preventing the network from learning under perfect conditions; that is, make it **harder** for the network to learn

A climbing analogy:

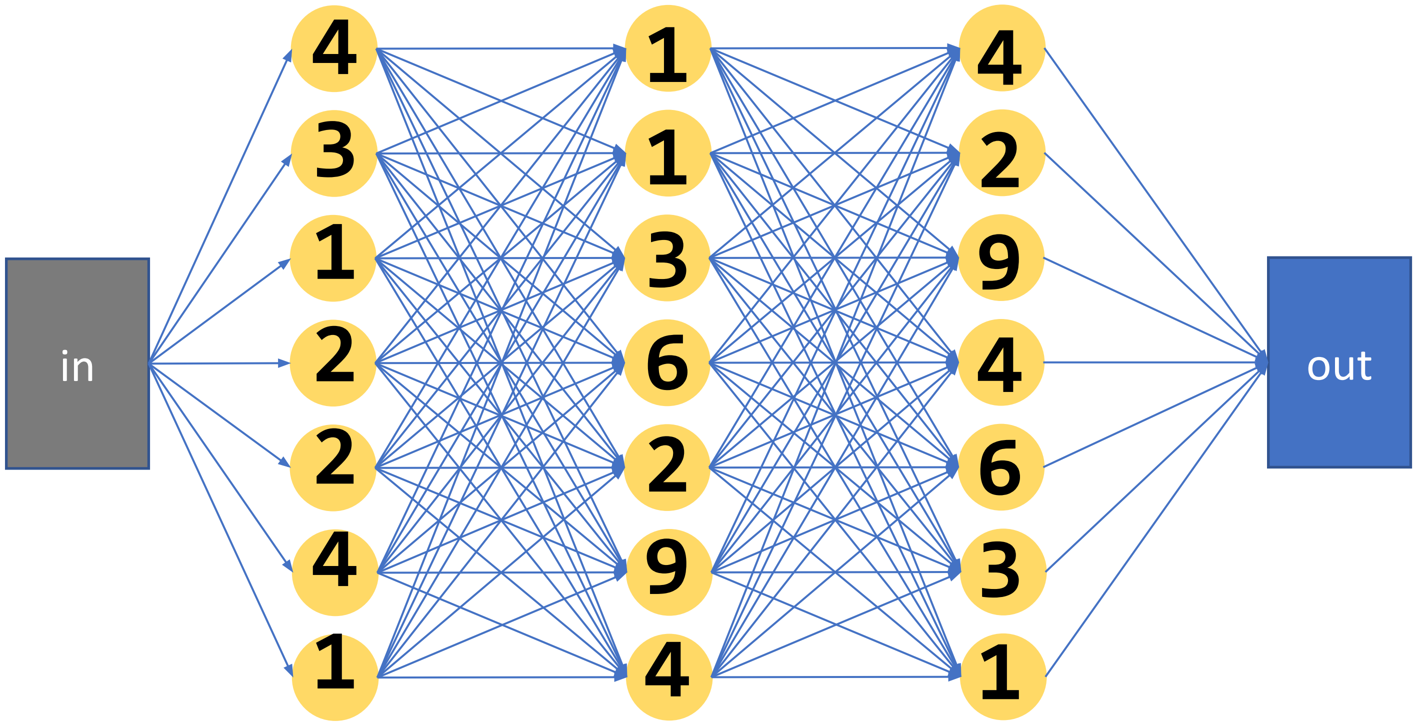
A person is climbing a wall using holds

- What if, I make a rule that she can climb
- … only using certain holds (say just green ones!)
- If she can learn to do this using fewer holds…
- …she'll definitely be able to do it with ALL the holds
- (learn better climbing techniques in the process)

Dropout ~= using only a certain holds instead of ALL the holds

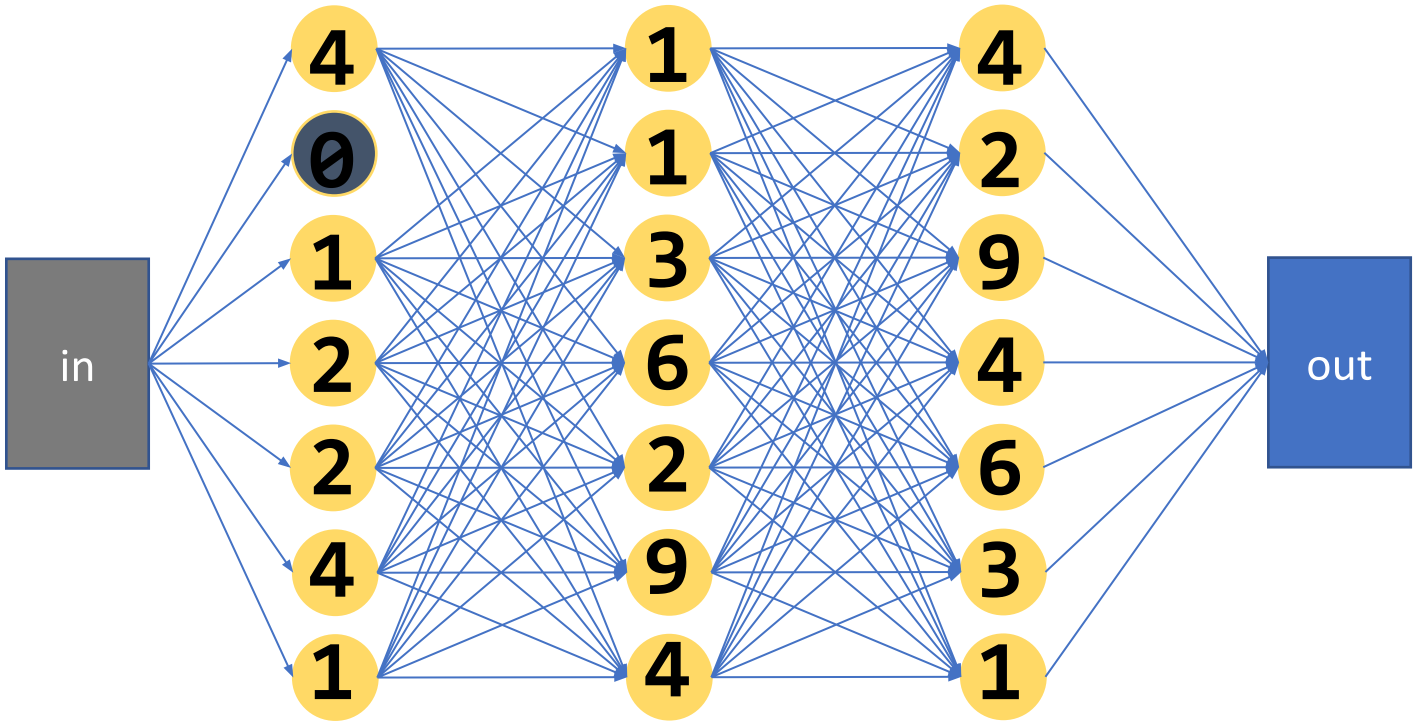
Image source https://www.istockphoto.com/illustrations/indoor-climbing

Dropout - what?



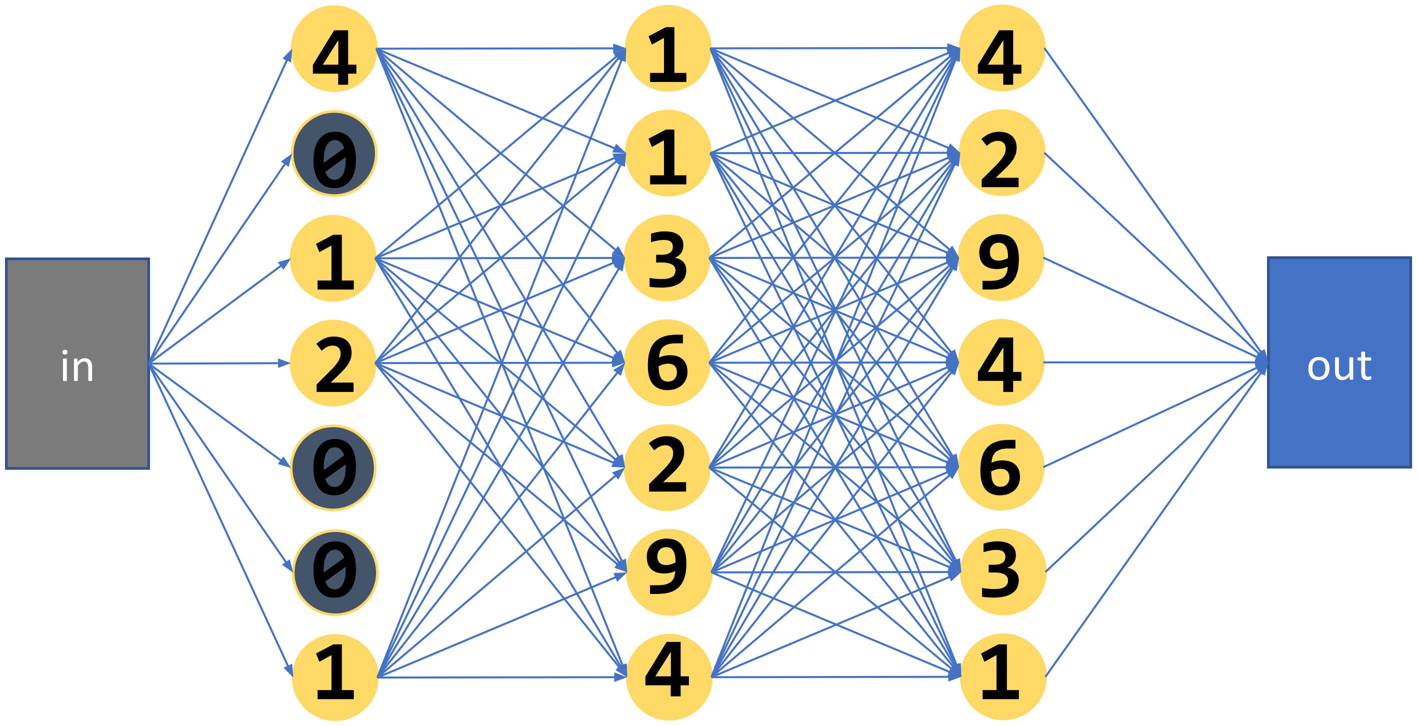
Typical NN: the output of every node in every layer is used in the next layer of the network

Dropout - what?



Dropout: *in a single training pass*, the output of randomly selected nodes from each layer will “drop out”, i.e. be set to 0

Dropout - what?



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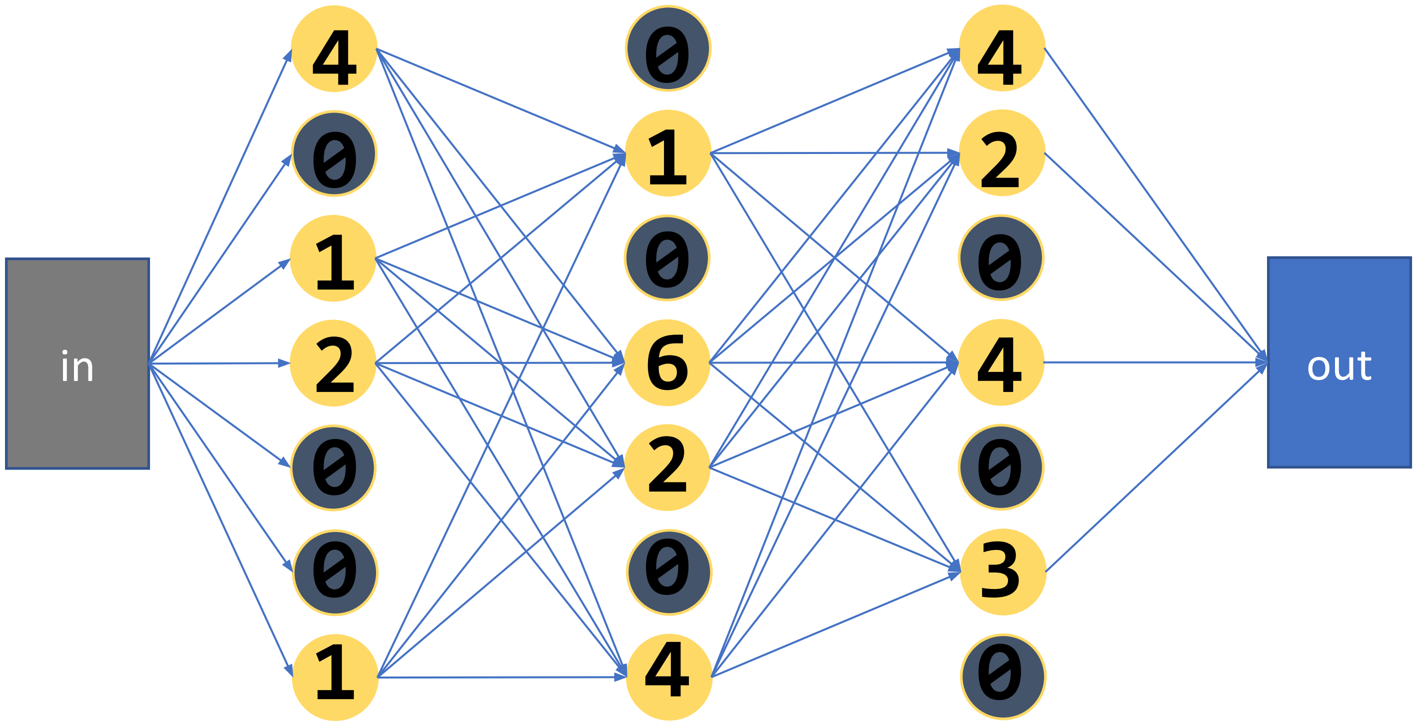
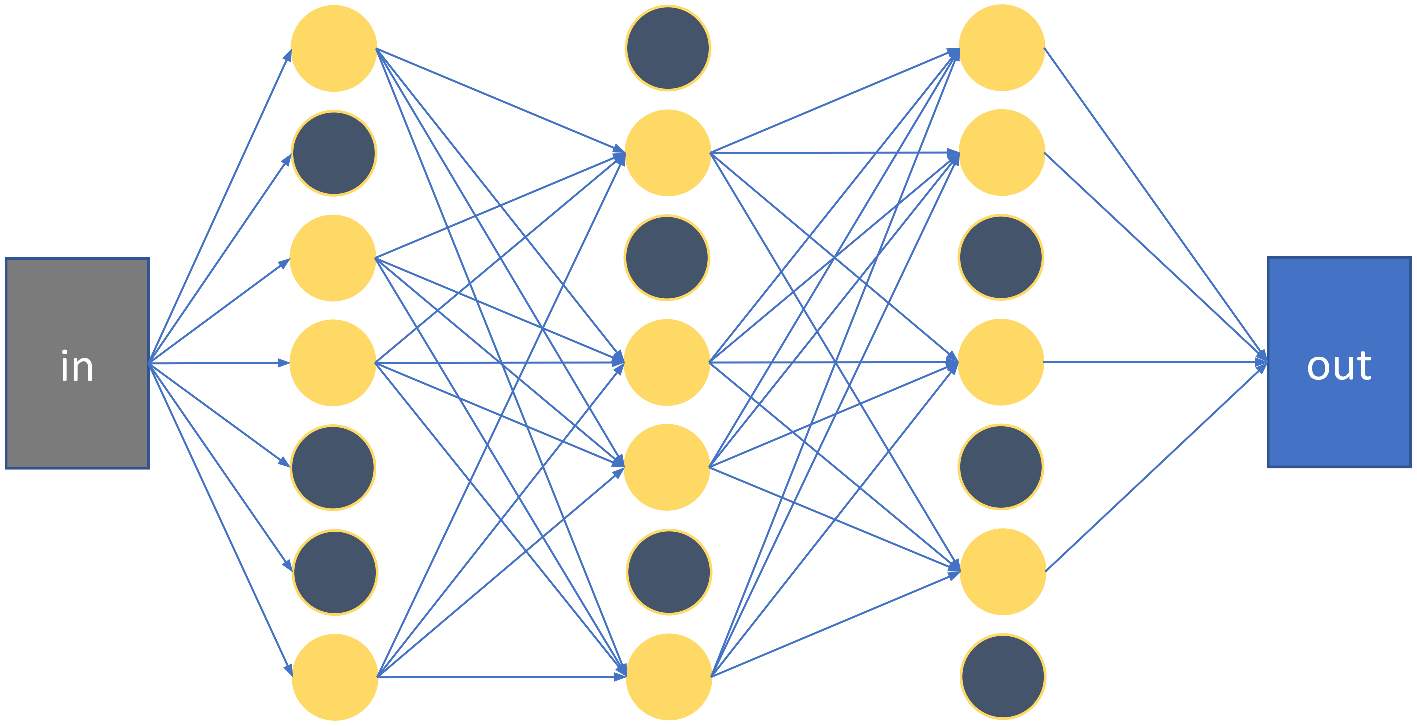


Not just limited to the input layer: can do this to *any* layer of the network

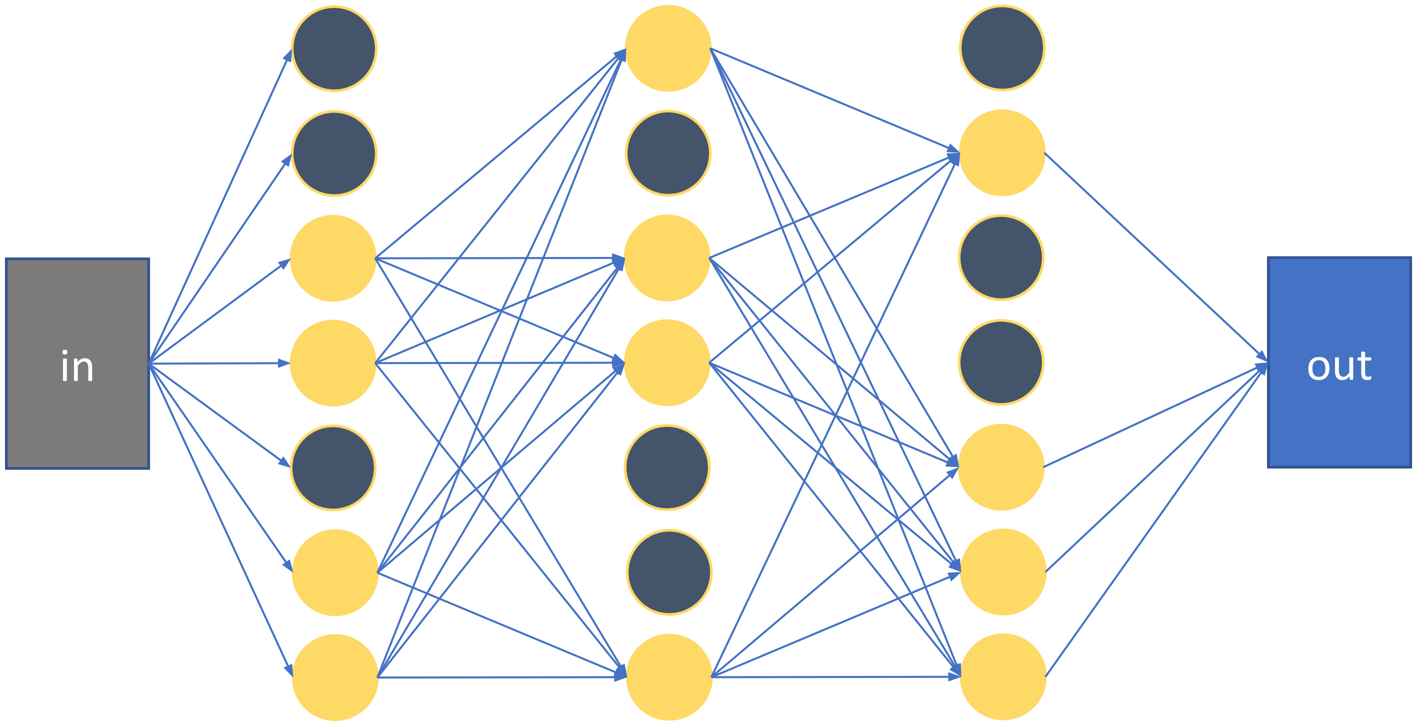
Dropout - what?



The nodes that drop out will be different each pass

(re-randomly selected)

Dropout - what?



The nodes that drop out will be different each pass

(re-randomly selected)

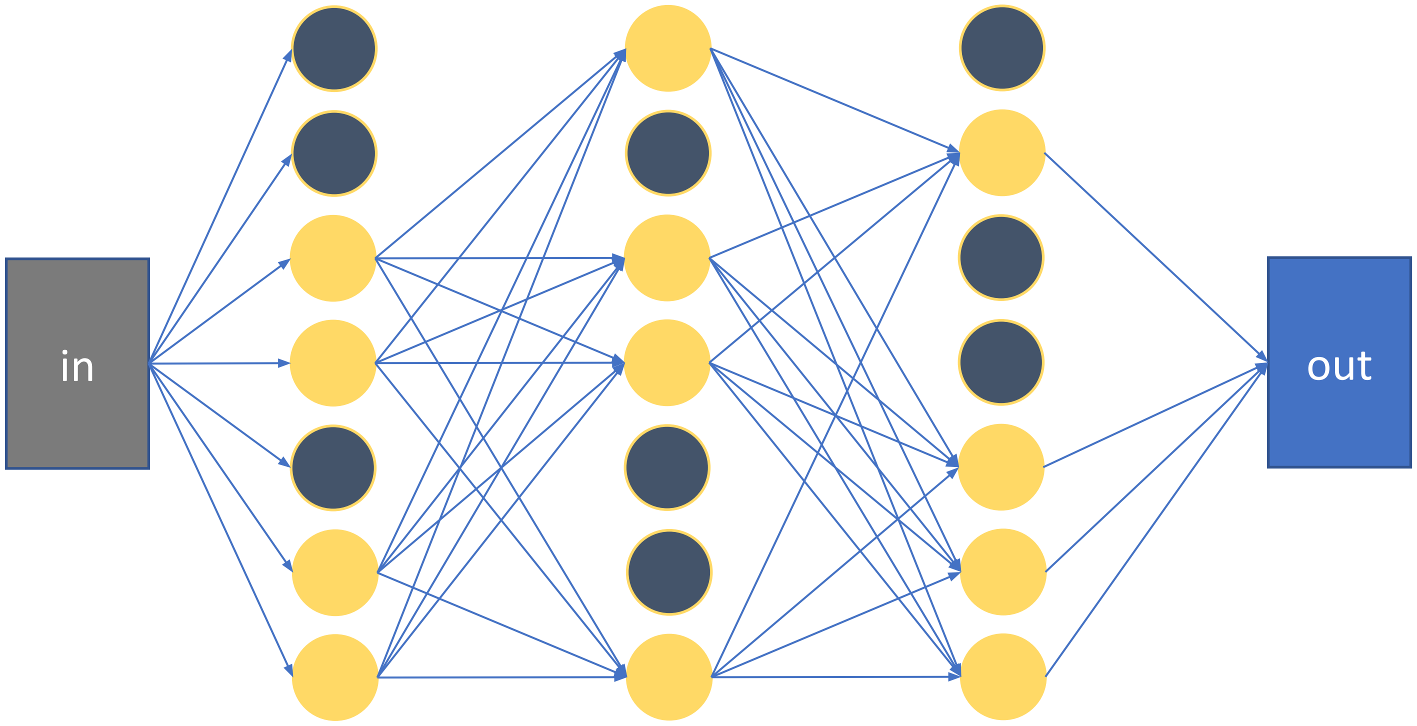
Dropout - why?

- Sort of looks like data augmentation, if you squint hard enough
  - Augmenting the data by randomly dropping out parts of it
- Over multiple passes through the net (i.e. during training over many epochs):
  - Randomly dropping neurons “forces” each neuron to learn a non-trivial weight
  - The network can’t learn to rely on spurious correlations (i.e. meaningless patterns), because they randomly might not be present

Do we use dropout while testing?

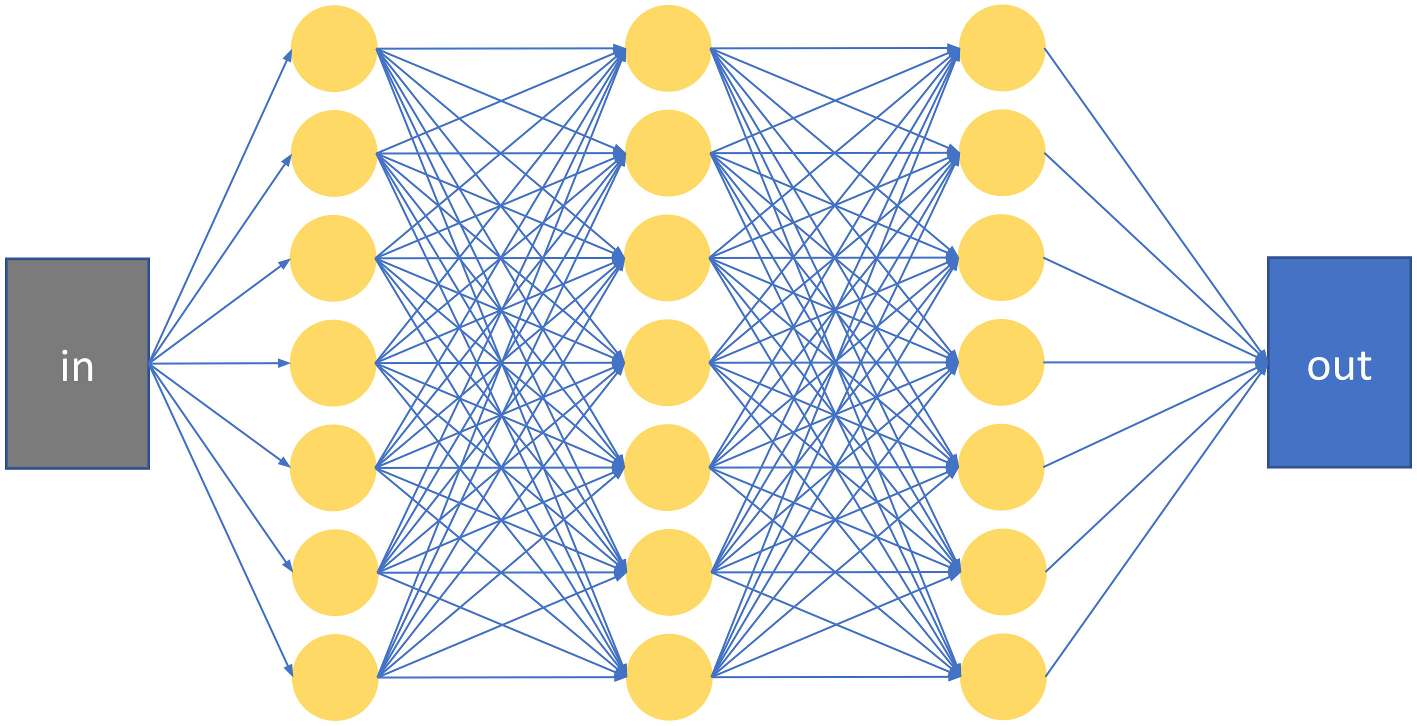
Why not?

Dropout: Implications for test time



- During testing, we stop dropping out and use all of the neurons again

Dropout: Implications for test time



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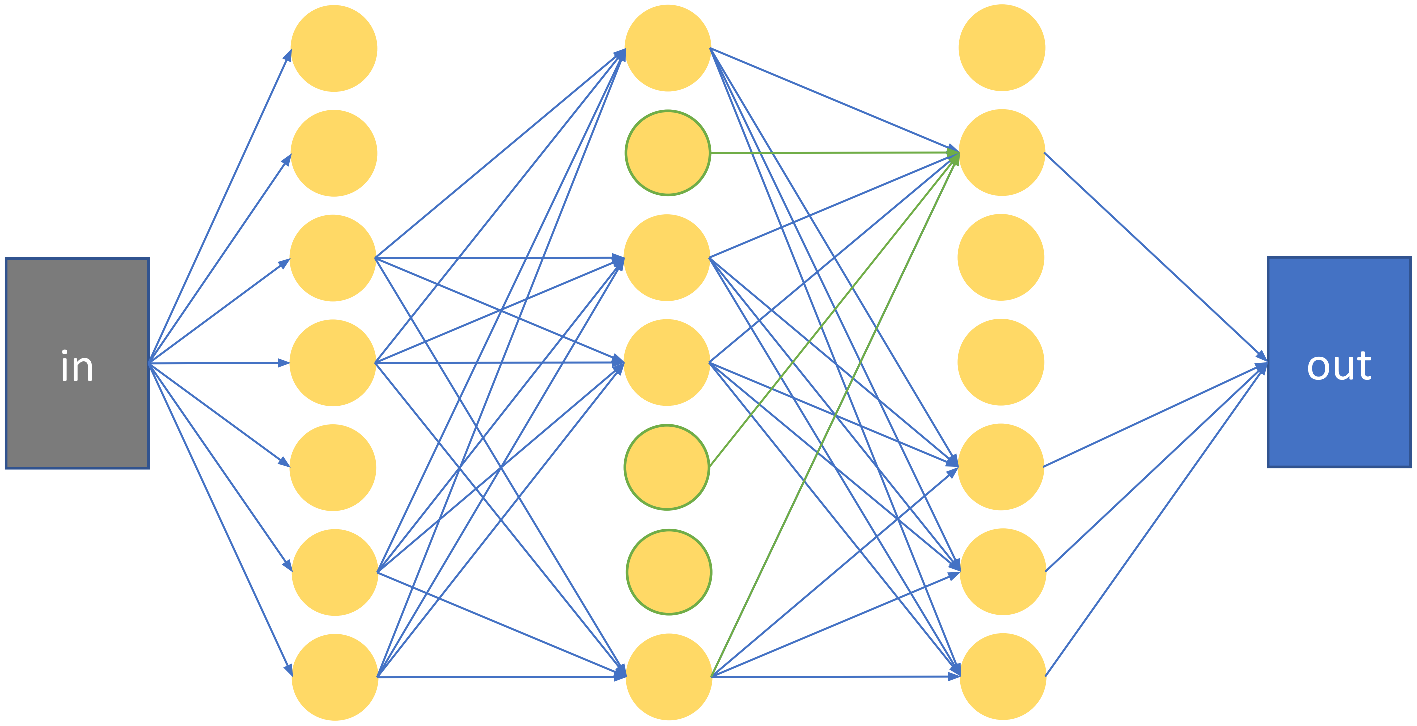
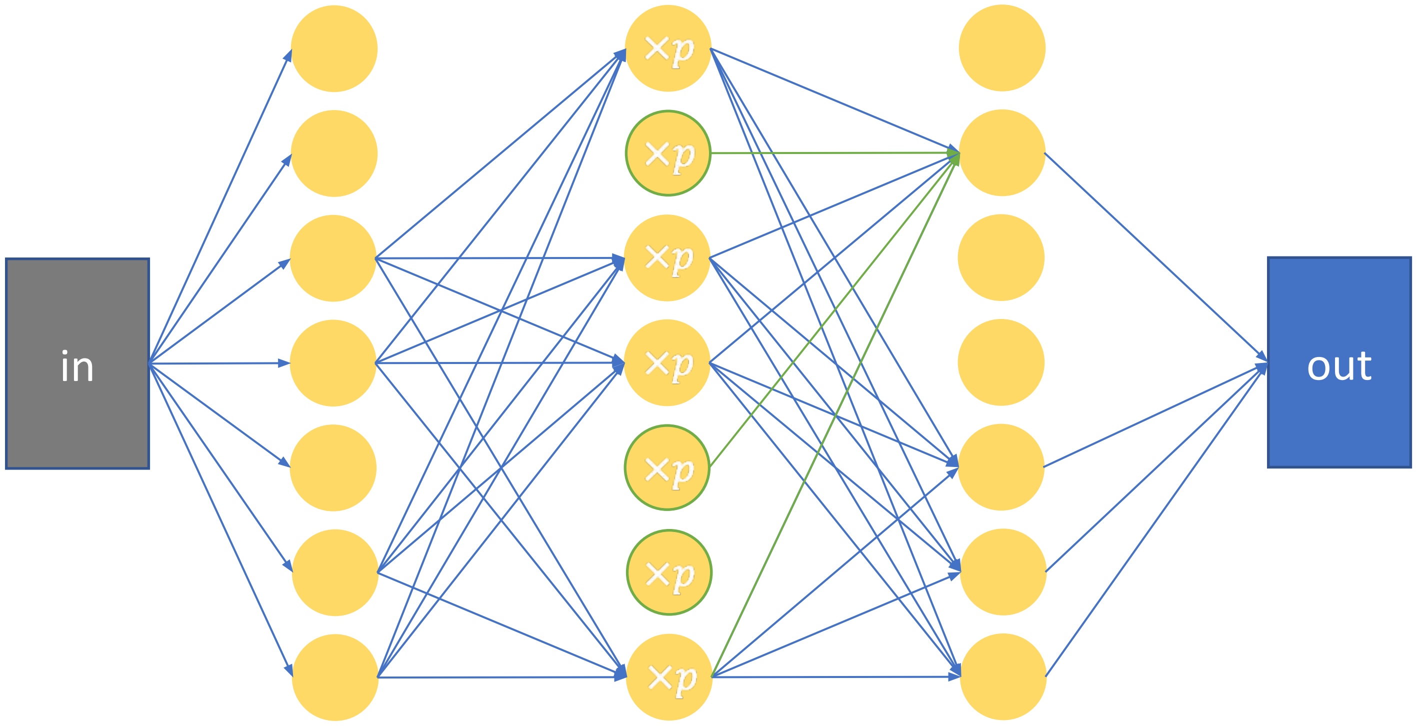
Dropout: Implications for test time



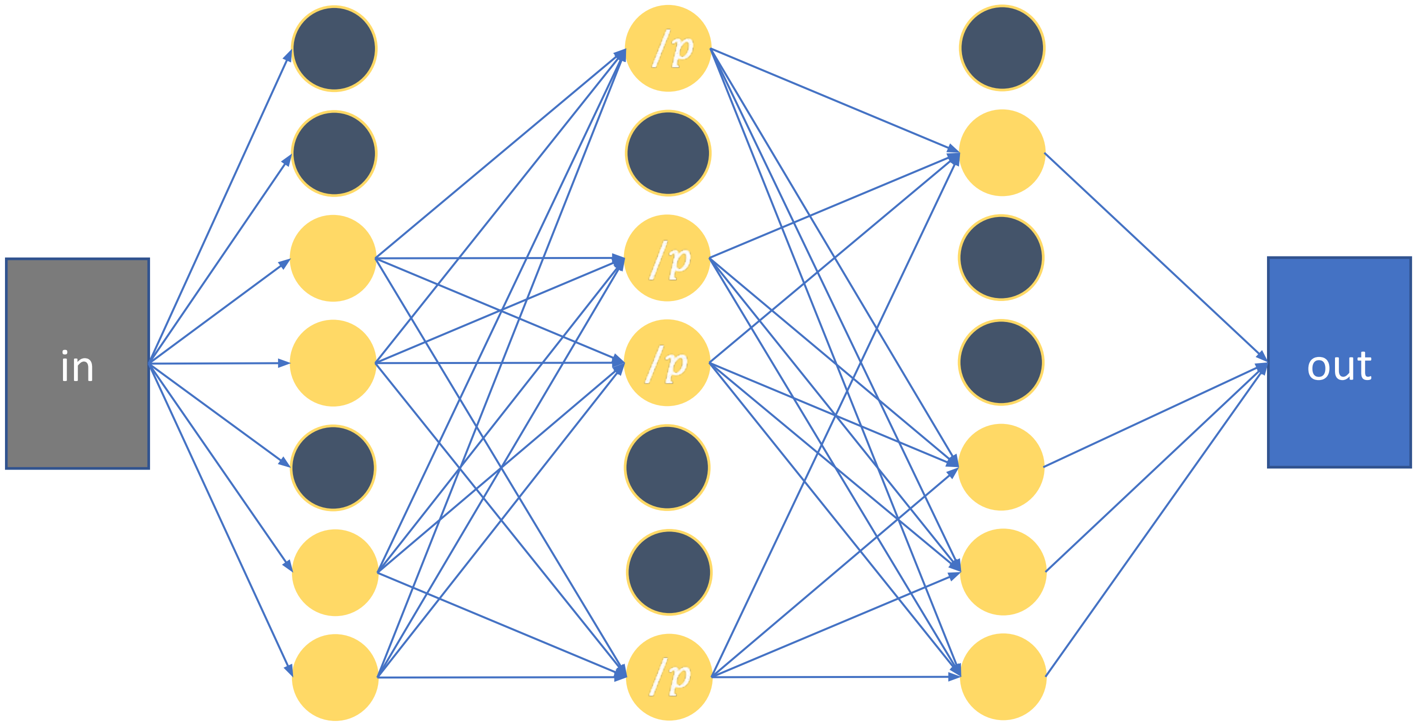
- During testing, we stop dropping out and use all of the neurons again
- If a layer keeps a fraction p of its neurons during training, then when we use all the neurons at test time, the next layer will get a bigger input than expected…
- ***What do we do!?***

Dropout: Implications for test time



- **Solution 1:**
  Multiply the values of all neurons by p, so that the expected magnitude of the sum of neurons is the same

Dropout: Implications for test time



- **Solution 1:**
  Multiply the values of all neurons by p, so that the expected magnitude of the sum of neurons is the same
- **Solution 2:**
  At training time, divide the values of the kept neurons by p

Dropout - implementation

- Handy keras layer!

- **`tf.keras.layers.Dropout(rate)`**
  - Hyperparameter `rate` between [0, 1]: the rate at which the outputs of the previous layer are dropped
  - **`Rate = 0.5`**: drop half, keep half
  - **`Rate = 0.25`**: drop ¼, keep ¾

Dropout - why not?

- It’s invasive to the network – we’re “reaching inside” and directly modifying it
- Might be nice if we could get similar benefits without having to modify the network itself...

Overfitting: What can we do about it?

1. Early stopping
2. Reduce parameters
3. Data augmentation
4. Dropout
5. **Regularization**

Regularization - why?

This approach leaves the network architecture unchanged, and instead only modifies the ***loss***.

- Adds an additional term to our existing loss function

Remember insight from before:

- Overfitting is correlated with the net relying **too heavily** on **too many *different*** correlations

Can we design a loss function that penalizes:

1. Heavy reliance on any correlation in the data?
2. Reliance on too many different correlations in the data?

Regularization - L1 vs L2

L2 regularization

- $\lambda \sum_{j=1}^{n} |W_j|^2$
- Penalize sum of squared weights
- **Effect**: keeps all weights small-ish, i.e. network can't learn to rely too heavily on any single pattern in the data

L1 regularization

- $\lambda \sum_{j=1}^{n} |W_j|$
- Penalize absolute value of weights
- **Effect**: tends to produce *sparse weights* (i.e. many zero-valued weights) → prevents the network from relying on too many different patterns in the data

For both, this is a term added to the existing loss function.

λ controls the strength of the penalty

Regularization - L1 vs L2

L1 Regularization

$$\text{Cost} = \sum_{i=0}^{N}\left(y_i - \sum_{j=0}^{M} x_{ij}W_j\right)^2 + \lambda \sum_{j=0}^{M} |W_j|$$

L2 Regularization

$$\text{Cost} = \underbrace{\sum_{i=0}^{N}\left(y_i - \sum_{j=0}^{M} x_{ij}W_j\right)^2}_{\text{Loss function}} + \lambda \underbrace{\sum_{j=0}^{M} W_j^2}_{\text{Regularization Term}}$$

Regularization: implementation

- Implementing yourself
  - When calculating loss - Get list of model parameters, take L1/L2 norm, multiply by lambda – add to loss.
- If you only want to regularize the weights of certain layers:
  In **`tf.keras`**, regularization can be passed as an argument to the layer constructor:
  - **`tf.keras.layers.Dense(16, kernel_regularizer=keras.regularizers.l1(lambda), activation='relu')`**

Putting it all together

- Demo

TL;DR – Rule of Thumb for Overfitting:

“Make start with the small-ish architecture and your net bigger until it starts to overfit...

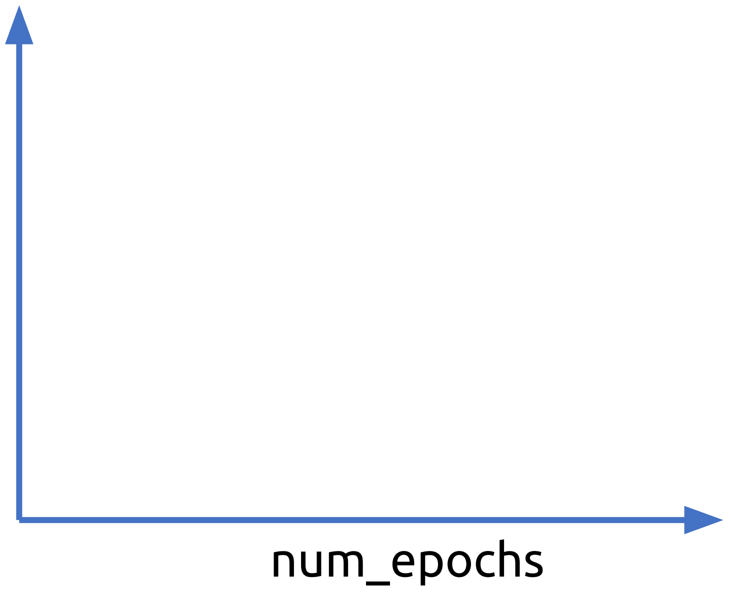
(use train/validation loss curves to monitor)

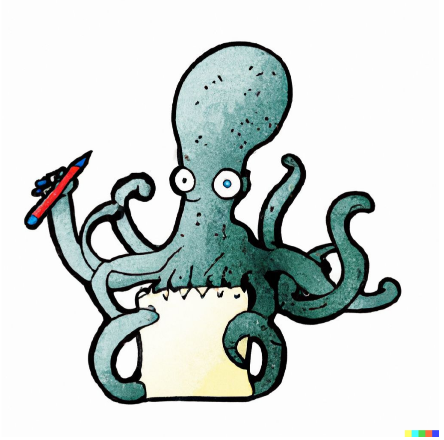
...then apply one of the techniques from this lecture”

Recap

Real-world data

- Messy and needs pre-processing
- Can lead to overfitting
- Early stopping may help but not the best solution





Handling overfitting

- Reduce parameters
- Data Augmentation
- Dropout
- Regularization

L1 Regularization

$$\text{Cost} = \sum_{i=0}^{N}(y_i - \sum_{j=0}^{M} x_{ij}W_j)^2 + \lambda \sum_{j=0}^{M} |W_j|$$

L2 Regularization

$$\text{Cost} = \underbrace{\sum_{i=0}^{N}(y_i - \sum_{j=0}^{M} x_{ij}W_j)^2}_{\text{Loss function}} + \underbrace{\lambda \sum_{j=0}^{M} W_j^2}_{\text{Regularization Term}}$$